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STRUCTURE FILE UPDATES: 1 AUG 2006 HIGHEST RN 897851-29-5
DICTIONARY FILE UPDATES: 1 AUG 2006 HIGHEST RN 897851-29-5

New CAS Information Use Policies; enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

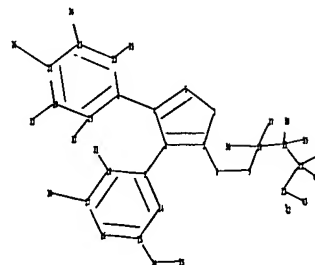
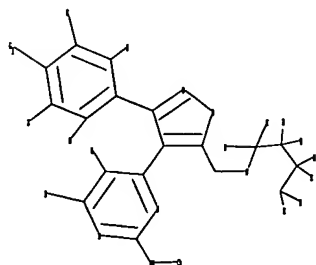
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10657811isoxazole.str



8 24 25 26 30 31 32 33 34 35 36 37 38 39 40 41 42 43

1	2	3	4	5	6	7	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
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2-8 3-7 4-6 8-9 10-36 10-37 11-12 11-38 11-39 12-40 12-41 13-42 13-43

15-24 17-30 18-31 19-32 20-33 21-26 22-34 23-35 24-25

1-2 1-5 2-3 3-4 4-5 6-19 6-23 7-14 7-18 9-10 10-11 12-13 14-15 15-16

16-17 17-18 19-20 20-21 21-22 22-23

exact/norm bonds :

4-5 8-9 9-10 10-11 12-13 15-24 21-26

exact bonds :

1-2 1-5 2-3 2-8 3-4 3-7 4-6 10-36 10-37 11-12 11-38 11-39 12-40 12-41

13-42 13-43 17-30 18-31 19-32 20-33 22-34 23-35 24-25

normalized bonds :

6-19 6-23 7-14 7-18 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23

isolated ring systems :

containing 1 : 6 : 7 : 9 : 10 : 11 : 12 : 13 :

G1:H, Cl, Br, F, I

Match level :

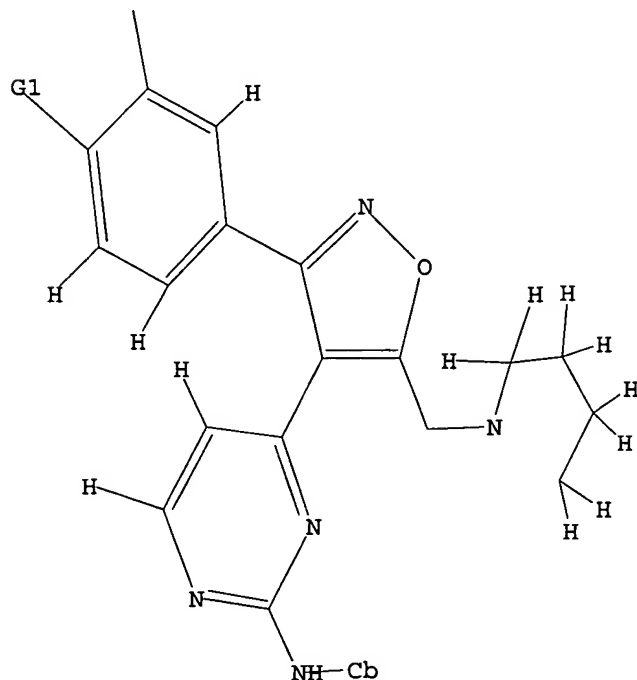
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:Atom 26:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS
```

L1 STRUCTURE UPLOADED

$$\Rightarrow d_{11}$$

L1 HAS NO ANSWERS

L1	STR
----	-----



G1 H, Cl, Br, F, I

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 15:37:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 3 TO 163

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 15:37:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> log hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 15:37:18 ON 03 AUG 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'REGISTRY' AT 15:39:04 ON 03 AUG 2006

FILE 'REGISTRY' ENTERED AT 15:39:04 ON 03 AUG 2006

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

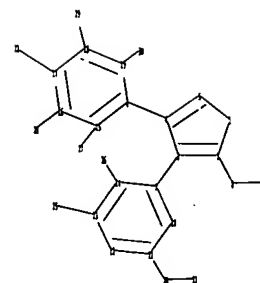
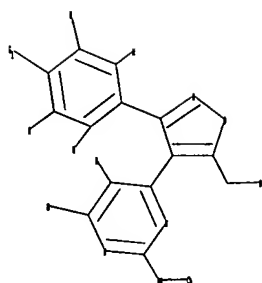
FULL ESTIMATED COST

166.94

167.15

=>

Uploading C:\Program Files\Stnexp\Queries\10657811isoxazole2.str



```

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ring nodes :
1 2 3 4 5 6 7 9 10 11 12 13 14 15 16 17 18 19
chain bonds :
2-8 3-7 4-6 8-9 11-20 13-25 14-26 15-27 16-28 17-22 18-29 19-30 20-21
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-15 6-19 7-10 7-14 10-11 11-12 12-13 13-14 15-16
16-17 17-18 18-19
exact/norm bonds :
4-5 8-9 11-20 17-22
exact bonds :
1-2 1-5 2-3 2-8 3-4 3-7 4-6 13-25 14-26 15-27 16-28 18-29 19-30 20-21
normalized bonds :
6-15 6-19 7-10 7-14 10-11 11-12 12-13 13-14 15-16 16-17 17-18 18-19
isolated ring systems :
containing 1 : 6 : 7 : 9 :

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G1:H,Cl,Br,F,I

Match level :

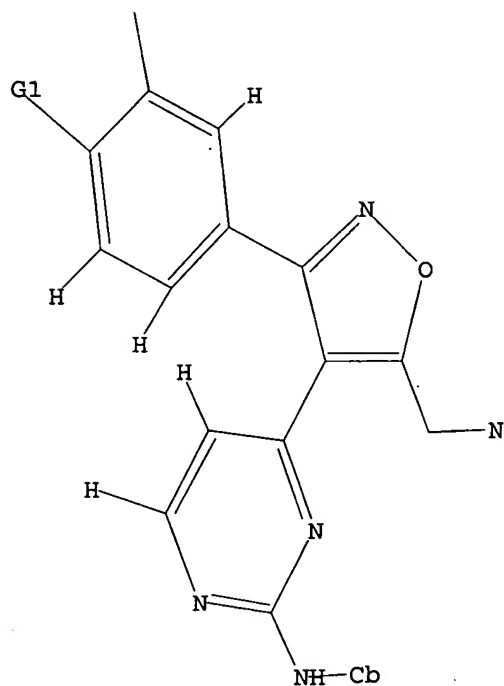
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20:CLASS 21:Atom 22:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS

L4 STRUCTURE UPLOADED

=> d l4

L4 HAS NO ANSWERS

L4 STR



G1 H, Cl, Br, F, I

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 15:39:27 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 3 TO 163

PROJECTED ANSWERS: 3 TO 163

L5 3 SEA SSS SAM L4

=> scan l5

ENTER FIELD CODE (BI):bi

E1 11 L4R/BI

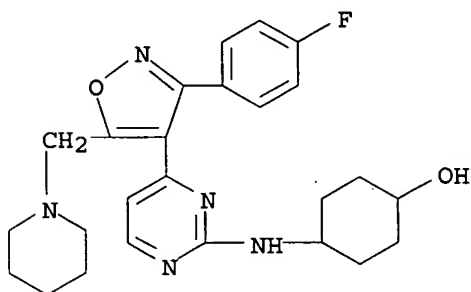
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E4	3	L5'/BI
E5	2	L5'HER13/BI
E6	20	L5.1/BI
E7	1	L5.2/BI
E8	1	L5.3/BI
E9	3	L5.4/BI
E10	26	L5.5/BI
E11	2	L5A/BI
E12	45	L50/BI

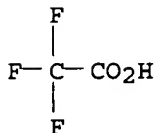
=> d 15 scan

L5 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Cyclohexanol, 4-[[4-[3-(4-fluorophenyl)-5-(1-piperidinylmethyl)-4-isoxazolyl]-2-pyrimidinyl]amino]-, mono(trifluoroacetate) (salt) (9CI)
 MF C25 H30 F N5 O2 . C2 H F3 O2

CM 1



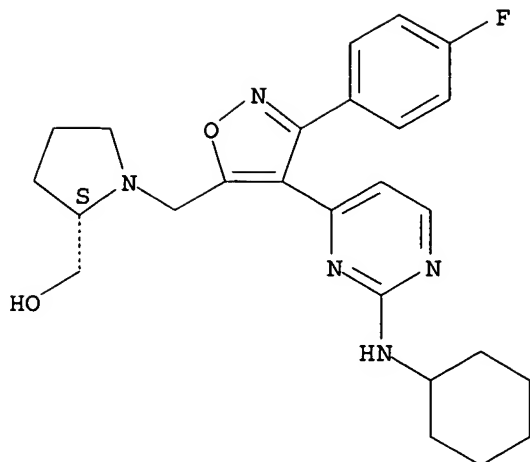
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

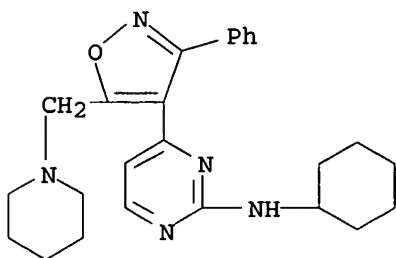
L5 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Pyrrolidinemethanol, 1-[[4-[2-(cyclohexylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, (2S)- (9CI)
 MF C25 H30 F N5 O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Pyrimidinamine, N-cyclohexyl-4-[3-phenyl-5-(1-piperidinylmethyl)-4-isoxazolyl]- (9CI)
 MF C25 H31 N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l4 sss full
 FULL SEARCH INITIATED 15:40:24 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 52 TO ITERATE

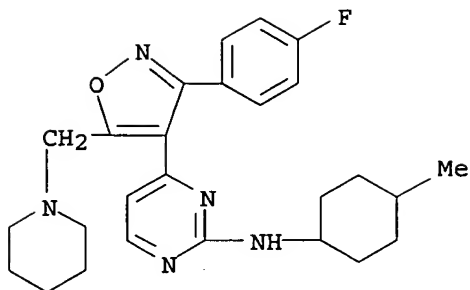
100.0% PROCESSED 52 ITERATIONS
 SEARCH TIME: 00.00.01

29 ANSWERS

L6 29 SEA SSS FUL L4

=> d l6 scan

L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Pyrimidinamine, 4-[3-(4-fluorophenyl)-5-(1-piperidinylmethyl)-4-isoxazolyl]-N-(4-methylcyclohexyl)- (9CI)
 MF C26 H32 F N5 O

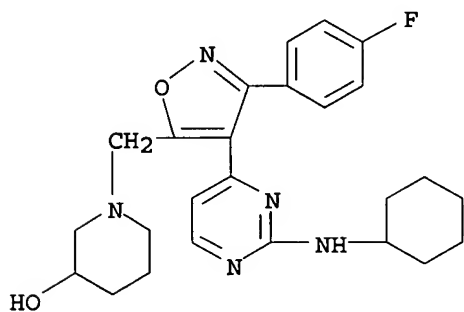


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

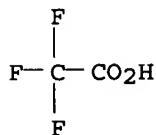
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 3-Piperidinol, 1-[[4-[2-(cyclohexylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, mono(trifluoroacetate) (salt) (9CI)
 MF C25 H30 F N5 O2 . C2 H F3 O2

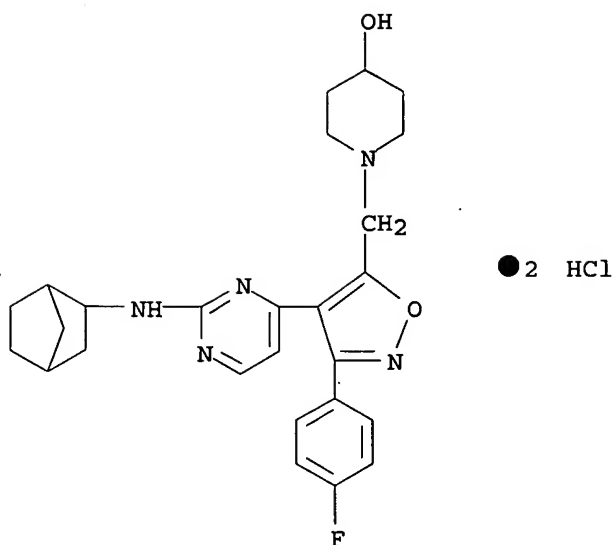
CM 1



CM 2

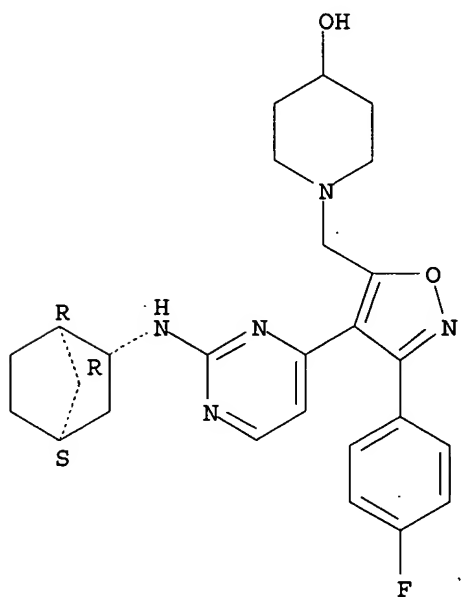


L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 4-Piperidinol, 1-[[4-[2-(bicyclo[2.2.1]hept-2-ylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, dihydrochloride (9CI)
 MF C26 H30 F N5 O2 . 2 Cl H



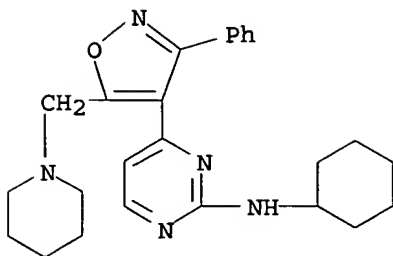
L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 4-Piperidinol, 1-[[4-[2-[(1R,2R,4S)-bicyclo[2.2.1]hept-2-ylamino]-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]- (9CI)
 MF C26 H30 F N5 O2
 CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 29 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Pyrimidinamine, N-cyclohexyl-4-[3-phenyl-5-(1-piperidin-1-ylmethyl)-4-isoxazolyl]- (9CI)
 MF C25 H31 N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> sel 16

E1 THROUGH E29 ASSIGNED

=> index bioscience paents

FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED

'PAENTS' IS NOT A VALID FILE NAME

ENTER A FILE NAME OR (IGNORE):patents

FILE 'ENCOMPAT2' ACCESS NOT AUTHORIZED

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
344.77	344.98

FULL ESTIMATED COST

INDEX 'ADISCTI, ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, ANTE, AQUALINE, AQUASCI, BIOENG, BIOSIS, BIOTECHABS, BIOTECHDS, BIOTECHNO, CABA, CAPLUS, CEABA-VTB, CIN, CONFSCI, CROPB, CROPU, DDFB, DDFU, DGENE, DISSABS, DRUGB, DRUGMONOG2, DRUGU, EMBAL, EMBASE, ...' ENTERED AT 15:41:41 ON 03 AUG 2006

92 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view search error messages that display as 0* with SET DETAIL OFF.

=> s E1-E29

2 FILE CAPLUS
30 FILES SEARCHED...
64 FILES SEARCHED...
68 FILES SEARCHED...
87 FILES SEARCHED...

1 FILES HAVE ONE OR MORE ANSWERS, 92 FILES SEARCHED IN STNINDEX

L7 QUE (326817-96-3/BI OR 673451-34-8/BI OR 673451-35-9/BI OR 673451-36-0/BI OR 673451-37-1/BI OR 673451-38-2/BI OR 673451-39-3/BI OR 673451-40-6/BI OR 673451-41-7/BI OR 673451-42-8/BI OR 673451-43-9/BI OR 673451-44-0/BI OR 673451-45-1/BI OR 673451-46-2/BI OR 673451-47-3/BI OR 673451-48-4/BI OR 673451-49-5/BI OR 673451-50-8/BI OR 673451-51-9/BI OR 673451-52-0/BI OR 673451-53-1/BI OR 673451-54-2/BI OR 673451-55-3/BI OR 673451-56-4/BI OR 673451-57-5/BI OR 673451-58-6/BI OR 673451-59-7/BI OR 673451-60-0/BI OR 673451-61-1/BI)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
1.22	346.20

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 15:43:08 ON 03 AUG 2006

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FILE COVERS 1907 - 3 Aug 2006 VOL 145 ISS 6
FILE LAST UPDATED: 1 Aug 2006 (20060801/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l6

L8 2 L6

=> d l8 1-2 ti abs bib

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

TI Preparation of isoxazoles and their use in the treatment of ischemic diseases

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H or halo; R2 = (un)substituted cycloalkyl; R3 for each occurrence independently = halo, alkyl, hydroxyalkyl, alkoxyalkyl, etc.; m = 0-2; n = 0-2] and their pharmaceutically acceptable salts are prepared and disclosed as useful for the treatment of neurol., neurodegenerative, ischemic and inflammatory disorders. Thus, e.g., II was prepared in 95% yield via substitution of 3-(4-fluorophenyl)-4-(3-methylsulfonylpyrimidin-4-yl)-5-(4-hydroxypiperidin-1-ylmethyl)isoxazole (preparation given) with cyclohexylamine. Preferred compds. of the invention demonstrated a protection value of $\geq 50\%$ in in vitro ischemia assay. Addnl., compds. were evaluated in in vitro CNS inflammation assays and preferred compds. possessed IC50 values of 300 nM or less. Accordingly, the invention also provides pharmaceutically acceptable compns. comprising the compds. of the invention and methods of utilizing those compds. and compns. in the treatment of neurol., neurodegenerative, ischemic and inflammatory disorders.

AN 2004:220330 CAPLUS

DN 140:270843

TI Preparation of isoxazoles and their use in the treatment of ischemic diseases

IN Ledebor, Mark; Ledford, Brian; Maltais, Francois

PA Vertex Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DT Patent

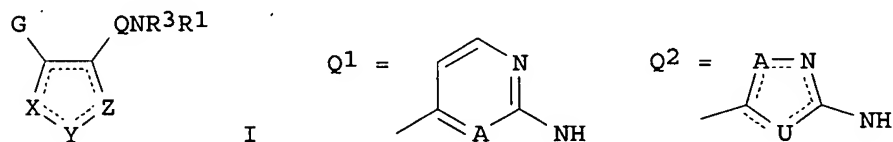
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI WO 2004022555 A1 20040318 WO 2003-US27903 20030908
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2003270350 A1 20040329 AU 2003-270350 20030908
US 2004132755 A1 20040708 US 2003-657811 20030908
EP 1546141 A1 20050629 EP 2003-752038 20030908
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JP 2006502168 T2 20060119 JP 2004-534669 20030908
PRAI US 2002-408813P P 20020906
WO 2003-US27903 W 20030908
OS MARPAT 140:270843
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
TI Preparation of as isoxazolylypyrimidines and related compounds as inhibitors of c-JUN N-terminal kinases and other protein kinases.
GI



AB Title compds. [I; XYZ = NOCR₂, ON:CR₂, N:NNR₃, OC(R₂):CR₂, NN(R₃)CR₂; R₁ = H, CONH₂, TnR, TnAr₂; R = (substituted) alipharyl; n = 0, 1; T = CO, CO₂, CONH, SO₂, SO₂NH, COCH₂, CH₂; R₂ = H, R, CH₂OR, CH₂OH, CHO, CH₂SR, CH₂SO₂R, CH₂NH₂, CH₂CN, (substituted) aryl, arylmethyl, heterocyclyl, heterocyclylmethyl, etc.; R₃ = H, R, COR, CO₂R, SO₂R; G = R, Ar₁; Ar₁ = (substituted) (fused) aryl, aralkyl, heterocyclyl; Q = Q₁, Q₂; A = N, CR₃; U = CR₃, O, S, NR₃; Ar₂ = (substituted) (fused) aryl, heterocyclyl], were prepared Thus, 4-(5-methyl-3-phenylisoxazole-4-yl)pyrimidin-2-ylamine (preparation given) was refluxed with PhBr, tris(dibenzylideneacetone)dipalladium, BINAP, and NaOCMe₃ were refluxed together for 16 h to give 36% 4-(5-methyl-3-phenylisoxazole-4-yl)pyrimidin-2-ylphenylamine. Several I inhibited K₂62 at <0.1 μM.
AN 2001:137207 CAPLUS
DN 134:178569
TI Preparation of as isoxazolylypyrimidines and related compounds as inhibitors of c-JUN N-terminal kinases and other protein kinases.
IN Green, Jeremy; Bemis, Guy; Grillot, Anne-Laure; Ledebor, Mark; Salituro, Francis; Harrington, Edmund; Gao, Huai; Baker, Christopher; Cao, Jingrong; Hale, Michael
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001012621	A1	20010222	WO 2000-US22445	20000811

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 CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
 HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
 LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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 US 1999-166922P P 19991122
 US 2000-211517P P 20000614
 WO 2000-US22445 W 20000811
 US 2002-74177 A3 20020212

OS MARPAT 134:178569

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 15:36:35 ON 03 AUG 2006)

FILE 'REGISTRY' ENTERED AT 15:36:45 ON 03 AUG 2006

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 L3 0 S L1 SSS FULL
 L4 STRUCTURE UPLOADED
 L5 3 S L4
 SCAN L5 BI
 L6 29 S L4 SSS FULL
 SEL L6

INDEX 'ADISCTI, ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, ANTE, AQUALINE,
 AQUASCI, BIOENG, BIOSIS, BIOTECHABS, BIOTECHDS, BIOTECHNO, CABA, CAPLUS,
 CEABA-VTB, CIN, CONFSCI, CROPB, CROPU, DDFB, DDFU, DGENE, DISSABS, DRUGB,
 DRUGMONOG2, DRUGU, EMBAL, EMBASE, ...' ENTERED AT 15:41:41 ON 03 AUG 2006
 SEA E1-E29

 2 FILE CAPLUS
 L7 QUE (326817-96-3/BI OR 673451-34-8/BI OR 673451-35-9/BI OR 6734

FILE 'CAPLUS' ENTERED AT 15:43:08 ON 03 AUG 2006

L8 2 S L6

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.94	352.14

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.50	-1.50

STN INTERNATIONAL LOGOFF AT 15:43:41 ON 03 AUG 2006